Cumene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 751 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.12e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

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Propylbenzene
Measured: 741
Predicted: 859

Image not found

Ethylbenzene
Measured: 170
Predicted: 271

Image not found

2,3,5-Trimethylphenol
Measured: 4070
Predicted: 345

Image not found

Naphthalene
Measured: 912
Predicted: 1250

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1,3,5-Trimethylbenzene
Measured: 661
Predicted: 493